

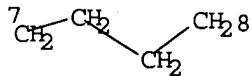
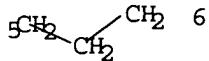
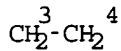
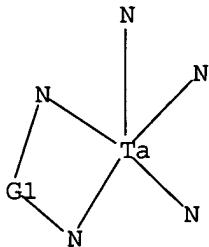
10/684,545

(FILE 'HOME' ENTERED AT 11:56:29 ON 01 MAR 2005)

FILE 'REGISTRY' ENTERED AT 11:56:46 ON 01 MAR 2005

L1 STRUCTURE uploaded
L2 STRUCTURE uploaded

=> d 12
L2 HAS NO ANSWERS
L2 STR



G1 N, Si, [@1-@2], [@3-@4], [@5-@6], [@7-@8]

Structure attributes must be viewed using STN Express query preparation.

=> s 12

SAMPLE SEARCH INITIATED 12:05:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 24 TO ITERATE

100.0% PROCESSED 24 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 187 TO 773

PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L2

=> s 12 full

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FULL SCREEN SEARCH COMPLETED - 448 TO ITERATE

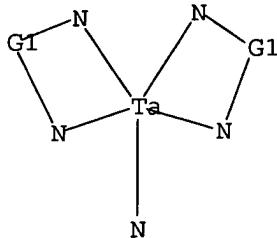
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SEARCH TIME: 00.00.01

L4 0 SEA SSS FUL L2

(FILE 'HOME' ENTERED AT 12:43:54 ON 01 MAR 2005)

FILE 'REGISTRY' ENTERED AT 12:44:14 ON 01 MAR 2005
L1 STRUCTURE uploaded

=> d 11
L1 HAS NO ANSWERS
L1 STR



G1 N, Si, CH2

Structure attributes must be viewed using STN Express query preparation.

=> s 12
L2 NOT FOUND

The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> s 11
SAMPLE SEARCH INITIATED 12:44:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 12 TO ITERATE

100.0% PROCESSED 12 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 33 TO 447
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full
FULL SEARCH INITIATED 12:44:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 278 TO ITERATE

100.0% PROCESSED 278 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

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FILE COVERS 1907 - 1 Mar 2005 VOL 142 ISS 10
FILE LAST UPDATED: 28 Feb 2005 (20050228/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s tantalum amide
85650 TANTALUM
117846 AMIDE
L1 17 TANTALUM AMIDE
(TANTALUM(W)AMIDE)

=> d 1-17 bib abs

L1 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:783724 CAPLUS
DN 141:424255
TI Zirconium, Hafnium, and **Tantalum Amide** Silyl Complexes: Their Preparation and Conversion to Metalla heterocyclic Complexes via γ -Hydrogen Abstraction by Silyl Ligands
AU Yu, Xianghua; Bi, Siwei; Guzei, Ilia A.; Lin, Zhenyang; Xue, Zi-Ling
CS Departments of Chemistry, University of Tennessee, Knoxville, TN, 37996-1600, USA
SO Inorganic Chemistry (2004), 43(22), 7111-7119
CODEN: INOCAJ; ISSN: 0020-1669
PB American Chemical Society
DT Journal
LA English
OS CASREACT 141:424255
AB New transition metal silyl amide complexes $(Me_2N)_3Ta[N(SiMe_3)_2](SiPh_2But)$ (1) and $[cyclic] (Me_2N)_3Ta[N(SiMe_3)_2]_2(SiPh_2But)$ ($M = Zr$, 2a, and Hf , 2b) were found to undergo γ -H abstraction by the silyl ligands to give metallaheterocyclic complexes $[cyclic] (Me_2N)_3Ta(NSiMe_3SiMe_2CH_2)$ (3) and $[cyclic] \{(Me_2N)_3Ta(NSiMe_3SiMe_2CH_2)\}_2$ ($M = Zr$, 4a, and Hf , 4b), resp. The conversion of 1 to 3 follows first-order kinetics with $\Delta H_{thermod.} = 23.6(1.6)$ kcal/mol and $\Delta S_{thermod.} = 3(5)$ eu between 288 and 313 K. The formation of 4a from $(Me_2N)_3Ta[N(SiMe_3)_2]_2Cl$ (5a) and $Li(THF)_2SiPh_2But$ (6) involves the formation of the intermediate 2a, followed by γ -H abstraction. Kinetic studies of these consecutive reactions, a second-order reaction to give 2a and then a first-order γ -H abstraction to give 4a, were conducted by an anal. method and a numerical method. At 278 K, the rate consts. k_1 and k_2 for the two consecutive reactions are $2.17(0.03) + 10^{-3} M^{-1} s^{-1}$ and $5.80(0.15) + 10^{-5} s^{-1}$ by the anal. method. The current work is a rare kinetic study of the $A + B \rightarrow C \rightarrow D (+ E)$ consecutive reactions. Kinetic studies of the formation of a metallaheterocyclic moiety $M(NSiMe_3SiMe_2CH_2)$ have not been reported. In addition, γ -H abstraction by a silyl ligand to give such a metallaheterocyclic moiety is new. Theor. investigations of the γ -H abstraction by silyl ligands have been conducted by d. functional theory calcns. at the Becke3LYP

(B3LYP) level, and they revealed that the formation of the metallacyclic complexes through γ -H abstraction is entropically driven. X-ray crystal structures of $(\text{Me}_2\text{N})_3\text{Ta}[\text{N}(\text{SiMe}_3)_2](\text{SiPh}_2\text{But})$ (1), $(\text{Me}_2\text{N})\text{Zr}[\text{N}(\text{SiMe}_3)_2]_2\text{Cl}$ (5a), and [cyclic] $\{(\text{Me}_2\text{N})[(\text{Me}_3\text{Si})_2\text{N}]\text{M}(\text{NSiMe}_3\text{SiMe}_2\text{C}\text{H}_2)\}_2$ ($\text{M} = \text{Zr}$, 4a, and Hf , 4b) are also reported.

RE.CNT 91 THERE ARE 91 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:784913 CAPLUS
DN 139:396019
TI Structure, Bonding, and Reactivity of Tantalum Amides Containing o-Naphthyl- and o-Indenylphenoxyde Ligation
AU Thorn, Matthew G.; Parker, Jennifer R.; Fanwick, Phillip E.; Rothwell, Ian P.
CS Department of Chemistry, Purdue University, West Lafayette, IN, 47907-2038, USA
SO Organometallics (2003), 22(23), 4658-4664
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
OS CASREACT 139:396019
AB The reaction of $[\text{Ta}(\text{NMe}_2)_5]$ with the o-(2,3-dihydro-1-naphthyl)-, o-(1-naphthyl)-, and o-(inden-3-yl)phenols $[\text{HO}\text{C}_6\text{H}_2\text{Ar-2-But}_2\text{-4,6}]$ ($\text{Ar} = \text{C}_10\text{H}_9$, C_10H_7 (Np), C_9H_7) has been investigated. In all three cases initial displacement of 1 equivalent of dimethylamine occurs, yielding mono(aryloxides) $[(\text{ArO})\text{Ta}(\text{NMe}_2)_4]$. Structural studies of the o-(2,3-dihydro-1-naphthyl) and o-(1-naphthyl) compds. 4 and 5 show they both adopt geometries best described as square pyramidal with an apical dimethylamido ligand and basal aryloxide oxygen. The Ta-O-Ar angles are 162° in both compds., with no metal interaction with the ortho substituents. Compound 4 reacts with 2,3,5,6-tetraphenylphenol to form the corresponding bis(aryloxide) 6. The intermediate o-(inden-3-yl)phenoxyde $[(\text{ArO})\text{Ta}(\text{NMe}_2)_4]$ 7 thermally eliminates a further 1 equivalent of HNMe_2 with formation of the tris(amido) compound $[\text{Ta}(\text{OC}_6\text{H}_2\{\eta^1\text{-Ind}\}-2\text{-But-4,6})(\text{NMe}_2)_3]$ 8. The coordination geometry about tantalum in 8 is best described as trigonal bipyramidal, with an oxygen and amido group in the axial positions: $\text{O-Ta-N} = 170^\circ$. The carbon atom of the indenyl ring bound directly to the phenoxyde nucleus is metalated, leading to a five-membered metallacycle. Hence, both deprotonation (CH bond activation) and tautomerization of the original inden-3-yl ring has occurred. The Ta-C(121) distance of $2.285(9)$ Å is consistent with an η^1 -indenyl ring being present in 8. Replacement of the dimethylamido ligands in 8 by chloride groups was achieved by reaction with SiCl_4 . Structural anal. of the 4-phenylpyridine adduct $[\text{Ta}(\text{OC}_6\text{H}_2\{\eta^3\text{-Ind}\}-2\text{-But-4,6})(\text{NC}_5\text{H}_4\text{Ph-4})\text{Cl}_3]$ 9 showed the presence of an η^3 -indenyl interaction with the tantalum metal center. The bonding parameters for the η^1 - and η^3 -indenyl rings are compared with those of related η^5 -cyclopentadienyl derivs. of niobium and tantalum.

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:613851 CAPLUS
DN 140:223914
TI Dinitrogen activation in sterically-hindered three-coordinate transition metal complexes
AU Christian, Gemma; Driver, Jenni; Stranger, Robert
CS Department of Chemistry, The Australian National University, Canberra, 0200, Australia
SO Faraday Discussions (2003), 124, 331-341
CODEN: FDISE6; ISSN: 1359-6640
PB Royal Society of Chemistry
DT Journal
LA English
AB Dinuclear metal systems based on sterically-hindered, three-coordinate transition metal complexes of the type ML_3 where the ancillary ligands L

comprise bulky organic substituents, hold great promise synthetically for the activation and scission of small, multiply-bonded mols. such as N2, NO and N2O. In this study we have employed d. functional methods to identify the metal/ligand combinations which achieve optimum activation and/or cleavage of N2. Strong π donor ligands such as NH2 and OH are found to produce the greatest level of activation based on N-N bond lengths in the intermediate dimer complex, L3Mo(μ -N2)MoL3, whereas systems containing the weak or non- π donor ligands NH3, PH3, OH2 and SH2 are found to be thermodynamically unfavorable for N2 activation. In the case of the Mo-NH2 and W-NH2 systems, a fragment bonding anal. reveals that the orientation of the amide ligands around the metal is important in determining both the spin state and the extent of dinitrogen activation in the intermediate dimer. For both systems, an intermediate dimer structure where one of the NH2 ligands on each metal is rotated 90° relative to the other ligands, is more activated than the structure in which the NH2 ligands are trigonally disposed around the metals. The level of activation is found to be very sensitive to the electronic configuration of the metal with d3 metal ions delivering the best activation along any one transition series. In particular, strong activation or cleavage of N2 was calculated for the third row d3 metals systems involving Ta(II), W(III) and Re(IVa), with the level of activation decreasing as the nuclear charge on the metal increases. This trend in activation reflects the size of the valence 5d orbitals and consequently, the capacity of the metal to back donate into the dinitrogen π^* orbitals.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:834154 CAPLUS
DN 138:205163
TI Competitive insertion of isocyanide into tantalum - amido and tantalum - methyl bonds
AU Amor, Francisco; Sanchez-Nieves, Javier; Royo, Pascual; Jacobsen, Heiko; Blacque, Olivier; Berke, Heinz; Lanfranchi, Maurizio; Pellinghelli, Maria Angela; Tiripicchio, Antonio
CS Departamento de Quimica Inorganica, Universidad de Alcala, Alcala de Henares, 28871, Spain
SO European Journal of Inorganic Chemistry (2002), (11), 2810-2817
CODEN: EJICFO; ISSN: 1434-1948
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
OS CASREACT 138:205163
AB The (amido)methyl complexes [Cp*Ta(NtBu)Me(NR2)] [Cp* = η 5-C5Me5; R = Ph (3), SiMe3 (4)] were prepared by reaction of [Cp*Ta(NtBu)ClMe] (1) with the appropriate lithium amides. Attempts to isolate the analogous NHMe derivative afforded a mixture of complexes [Cp*Ta(NtBu)Me(NHMe)] (5) and [Cp*Ta(NMe)Me(NHtBu)] (6), resulting from hydrogen exchange between the amido and imido ligands. Complexes 5 and 6 are not interconverting in THF solution in NMR time scale. Insertion of CN(2,6-Me2C6H3) into the Ta-Me bond of complexes 3 and 4 gave the η 1-iminoacyl derivs. [Cp*Ta(NtBu)(NR2){ η 1-C(Me)=N(2,6-Me2C6H3)}] [R = Ph (7), SiMe3 (8)]. The same reaction of the complexes [Cp*Ta(NtBu)Me(NRMe)] [R = H (5), Me (2)] proceeds as insertion into the Ta-NRMe bond and gave the η 2-iminocarbamoyl compds. [Cp*Ta(NtBu)Me{ η 2-C(NRMe)=N(2,6-Me2C6H3)}] (10, 9, resp.). All of the new compds. were characterized by 1H and 13C NMR spectroscopy. The x-ray crystal structure of 9 is reported. DFT calcns. were carried out to justify the preference of the insertion either into the Ta-C or the Ta-N bond.

RE.CNT 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:617671 CAPLUS
TI Synthesis and characterization of a tantalum amide hydride complex from the reaction of a tantalum amide with silane
AU Cai, Hu; Chen, Tianniu; Xue, Zi-Ling

CS Department of Chemistry, University of Tennessee, Knoxville, TN, 37996-1600, USA
SO Abstracts of Papers, 224th ACS National Meeting, Boston, MA, United States, August 18-22, 2002 (2002), INOR-519 Publisher: American Chemical Society, Washington, D. C.
CODEN: 69CZPZ
DT Conference; Meeting Abstract
LA English
AB The reaction of $[(Me_2N)_3TaCl_2]_2$ with $LiN(SiMe_3)_2$ yields $(Me_2N)_3Ta[\mu-CH_2Si(Me)_2NSiMe_3]$ (1) quant. 1 was found to react with H_3SiPh to yield dinuclear tantalum amido hydride 2. Our studies of these reactions and characterization of 1 and 2 are presented.

L1 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:639421 CAPLUS
TI New amide silyl and disilyl complexes of tantalum(V)
AU Xue, Ziling; Wu, Zhongzhi; Diminnie, Jonathon B.
CS Department of Chemistry, University of Tennessee, Knoxville, TN, 37996, USA
SO Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, United States, August 26-30, 2001 (2001), INOR-234 Publisher: American Chemical Society, Washington, D. C.
CODEN: 69BUZP
DT Conference; Meeting Abstract
LA English
AB **Tantalum amide silyl and bis(silyl) complexes**
 $(Me_2N)_3Ta(SiR_3)Cl$ [$SiR_3=Si(SiMe_3)_3$ (1), $SiPh_2But$ (2)], $(Me_2N)_4Ta(SiR_3)$ [$SiR_3=Si(SiMe_3)_3$ (3), $SiPh_2But$ (4)], $(Me_2N)_3Ta(SiPh_2But)_2$ (5), and $(Me_2N)_3Ta(SiPh_2But)[Si(SiMe_3)_3]$ (6) have been prepared and characterized. 3 reacts with one equiv of O_2 to give $(Me_2N)_3Ta(\eta^2-ONMe_2)[OSi(SiMe_3)_3]$ (7). The spectroscopic data of 1-6 and crystal structures of 1, 2 and 4 reveal that the coordination geometry around Ta atoms is trigonal bipyramidal with silyl ligands in the equatorial position in 1-4 and in the axial position in 5-6, resp.

L1 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:541456 CAPLUS
DN 135:331512
TI Synthesis of isomeric B-methylated tantalum carboranes, $(Me_2N)_3TaC_2B_9H_{10}Me$
AU Fox, Mark A.; Howard, Judith A. K.; Hughes, Andrew K.; Malget, John M.; Yufit, Dimitrii S.
CS Department of Chemistry, University of Durham, Durham, DH1 3LE, UK
SO Journal of the Chemical Society, Dalton Transactions (2001), (15), 2263-2269
CODEN: JCSDAA; ISSN: 1472-7773

PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 135:331512
AB The cage-alkylated metallacarborane complex $[4,4,4-(NMe_2)_3-3-Me-4,1,2-closo-TaC_2B_9H_{10}]$ (8), was obtained as the only product from the reaction of $Ta(NMe_2)_5$ with nido-11-Me-2,7-C₂B₉H₁₂, which is prone to skeletal rearrangement under basic conditions. That no rearrangement occurs indicates that the hydroaminolysis reaction is a clean synthetic method. The isomeric metallacarboranes $[3,3,3-(NMe_2)_3-4-Me-3,1,2-closo-TaC_2B_9H_{10}]$ (9) and $[2,2,2-(NMe_2)_3-3-Me-2,1,7-closo-TaC_2B_9H_{10}]$ (10) were produced from the reaction of $Ta(NMe_2)_5$ with $[Me_3NH]$ [nido-9-Me-7,8-C₂B₉H₁₁] and $[Me_3NH]$ [nido-8-Me-7,9-C₂B₉H₁₁], resp. Identities of the metallacarboranes 8, 9 and 10 were deduced by detailed multinuclear (¹¹B, ¹³C and ¹H) NMR spectroscopy. These geometries are supported by B NMR shift predictions based on observed shifts of the known non-methylated analogs $[3,3,3-(NMe_2)_3-closo-3,1,2-TaC_2B_9H_{10}]$ and $[3,3,3-(NMe_2)_3-closo-2,1,7-TaC_2B_9H_{10}]$ and calculated shifts (GIAO-B3LYP/6-311G*//MP2/6-31G*) of the B-Me carboranes, closo-3-Me-1,2-C₂B₁₀H₁₁, 4-Me-1,2-C₂B₁₀H₁₁ and 2-Me-1,7-C₂B₁₀H₁₁. The mol. structure of 8 was determined by x-ray diffraction.

RE.CNT 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:194211 CAPLUS
DN 135:19719
TI Insertion of carbon dioxide and isocyanide into **tantalum-amide** and tantalum-methyl bonds
AU Sanchez-Nieves, J.; Royo, P.
CS Departamento de Quimica Inorganica, Facultad de Ciencias, Campus Universitario, Universidad de Alcala, Alcala de Henares, E-28871, Spain
SO Journal of Organometallic Chemistry (2001), 621(1-2), 299-303
CODEN: JORCAI; ISSN: 0022-328X
PB Elsevier Science S.A.
DT Journal
LA English
OS CASREACT 135:19719
AB The Me-amide complex $[\text{TaCp}^*(\text{NtBu})\text{Me}(\text{NMe}_2)]$ (1a) was isolated by reaction of the chloro-Me $[\text{TaCp}^*(\text{NtBu})\text{MeCl}]$ complex with LiNMe_2 . Reaction of the mono-amide compds. $[\text{TaCp}^*(\text{NtBu})\text{XY}]$ ($\text{X} = \text{NMe}_2$, $\text{Y} = \text{Me}$ (1a); $\text{X} = \text{NHtBu}$, $\text{Y} = \text{Me}$ (1b), Cl (1c)) with CO_2 gives the η^2 -carbamate derivs. $[\text{TaCp}^*(\text{NtBu})(\eta^2\text{-O}_2\text{CX})\text{Y}]$ ($\text{X} = \text{NMe}_2$, $\text{Y} = \text{Me}$ (2a); $\text{X} = \text{NHtBu}$, $\text{Y} = \text{Me}$ (2b), Cl (2c)). A similar reaction with the di-amide complex $[\text{TaCp}^*(\text{NtBu})(\text{NHtBu})_2]$ (1d) gives the di-carbamate derivative $[\text{TaCp}^*(\text{NtBu})\{\eta^2\text{-O}_2\text{C}(\text{NHtBu})\}\{\eta^1\text{-O}_2\text{C}(\text{NHtBu})\}]$ (2d). Reaction of the Me-carbamate (2a) with isocyanide CNAr ($\text{Ar} = 2,6\text{-Me}_2\text{C}_6\text{H}_3$) gives the η^2 -iminoacyl- η^1 -carbamate complex $[\text{TaCp}^*(\text{NtBu})\{\eta^2\text{-C}(\text{Me})\text{:NAr}\}\{\eta^1\text{-O}_2\text{C}(\text{NMe}_2)\}]$ (3a). Formation of the related compound $[\text{TaCp}^*(\text{NtBu})\{\eta^2\text{-C}(\text{Me})\text{:NAr}\}\{\eta^1\text{-O}_2\text{C}(\text{NHtBu})\}]$ (3b) was only detected by NMR spectroscopy in C_6D_6 or CDCl_3 whereas the reaction of 2b in hexane gives the η^1 -iminoacyl- η^2 -carbamate complex $[\text{TaCp}^*(\text{NtBu})\{\eta^1\text{-C}(\text{Me})\text{:NAr}\}\{\eta^2\text{-O}_2\text{C}(\text{NHtBu})\}]$ (3b').

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

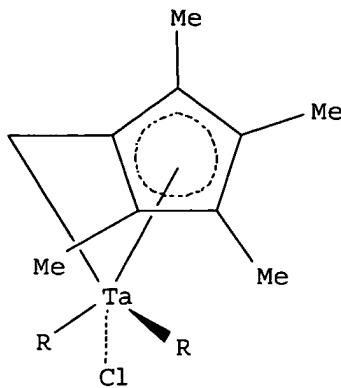
L1 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:732659 CAPLUS
DN 134:100959
TI Insertion and cleavage reactions of $[\text{closo-3,1,2-Ta}(\text{NMe}_2)_3(\text{C}_2\text{B}_9\text{H}_{11})]$ with nitriles, phenols and thiols; structural characterization of N,N-dimethylamidinate ligands
AU Broder, Charlotte K.; Goeta, Andres E.; Howard, Judith A. K.; Hughes, Andrew K.; Johnson, Andrew L.; Malget, John M.; Wade, Ken
CS Department of Chemistry, University Science Laboratories, Durham, DH1 3LE, UK
SO Dalton (2000), (20), 3526-3533
CODEN: DALTFG
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 134:100959
AB The Ta complex $[\text{closo-3,1,2-Ta}(\text{NMe}_2)_3(\text{C}_2\text{B}_9\text{H}_{11})]$ underwent insertion into the N-Ta bond by MeCN and p-fluorobenzonitrile to give the N,N-dimethylacetamidinate complex $[\text{closo-3,1,2-Ta}\{\text{N:C}(\text{Me})\text{NMe}_2\}_3(\text{C}_2\text{B}_9\text{H}_{11})]$, and p-fluoro-N,N-dimethylbenzamidinate complex, $[\text{closo-3,1,2-Ta}\{\text{N:C}(\text{C}_6\text{H}_4\text{F})\text{NMe}_2\}_3(\text{C}_2\text{B}_9\text{H}_{11})]$, resp. Attempted recrystn. of the latter from chlorinated solvents led to $[\text{closo-3,1,2-Ta}\{\text{N:C}(\text{C}_6\text{H}_4\text{F})\text{NMe}_2\}_2\text{Cl}(\text{C}_2\text{B}_9\text{H}_{11})]$, in which one amidinate ligand was replaced by a chloride. $[\text{closo-3,1,2-Ta}(\text{NMe}_2)_3(\text{C}_2\text{B}_9\text{H}_{11})]$ reacts with cyclohexyl isocyanide to give $[\text{Ta}(\text{NMe}_2)_2\{\eta^2\text{-N}(\text{Cy})\text{CNMe}_2\}(\text{C}_2\text{B}_9\text{H}_{11})]$. The structures of the novel N,N-dialkylamidinate complexes were determined by single crystal x-ray diffraction, and reveal the extensive delocalization and strong π -donor character of the amidinate ligands. The M-N bonds of $[\text{closo-3,1,2-Ta}(\text{NMe}_2)_3(\text{C}_2\text{B}_9\text{H}_{11})]$ are cleaved by protic reagents, and it reacts with 2,6-dimethylphenol to give $[\text{closo-3,1,2-Ta}(\text{OC}_6\text{H}_3\text{Me}_2-2,6)_3(\text{C}_2\text{B}_9\text{H}_{11})]$ and with benzenethiol to give the charge-compensated complex $[\text{closo-3-Ta}(\text{SC}_6\text{H}_5)_4(9\text{-NHMe}_2-1,2\text{-C}_2\text{B}_9\text{H}_{10})]$ where the $\beta\text{-B}$ of the C_2B_3 face bears an NHMe_2^+ substituent. The structures of the last two compds. also were determined by x-ray crystallog.

RE.CNT 80 THERE ARE 80 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:688374 CAPLUS
DN 132:122706
TI Transition metal dicarbollide complexes: synthesis, molecular, crystal and electronic structures of $[M(C_2B_9H_{11})(NMe_2)_3]$ ($M = Nb$ or Ta) and their insertion reactions with CO_2 and CS_2
AU Batsanov, Andrei S.; Churakov, Andrei V.; Howard, Judith A. K.; Hughes, Andrew K.; Johnson, Andrew L.; Kingsley, Andrew J.; Neretin, Ivan S.; Wade, Ken
CS Department of Chemistry, University of Durham, Durham, DH1 3LE, UK
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1999), (21), 3867-3875
CODEN: JCDTBI; ISSN: 0300-9246
PB Royal Society of Chemistry
DT Journal
LA English
AB The homoleptic amides $[M(NMe_2)_5]$ ($M = Nb$ 1 or Ta 2; the latter is characterized by a structural study) reacted with the carborane nido- $C_2B_9H_{13}$ to eliminate two equivalent of $HNMe_2$ and generate the dicarbollide half-sandwich tris(dimethylamide) complexes $[M(C_2B_9H_{11})(NMe_2)_3]$ ($M = Nb$ 3 or Ta 4). The crystal structures of isomorphous 3 and 4 were determined and reveal two NMe_2 ligands in a vertical orientation and the 3rd one in a horizontal orientation with respect to the η^5 -coordinated face of the $C_2B_9H_{11}$ ligand. The electronic factors responsible for the amide ligand orientations in these complexes are explored using qual. MO arguments. Complexes 3 and 4 reacted with CO_2 and CS_2 to yield the tris(carbamate) $[M(C_2B_9H_{11})(O_2CNMe_2)_3]$ ($M = Nb$ 5 or Ta 7) and tris(dithiocarbamate) $[M(C_2B_9H_{11})(S_2CNMe_2)_3]$ ($M = Nb$ 6 or Ta 8) complexes, resp. The crystal structures of 6 and 7 show two (dithio)carbamate ligands in horizontal and one in vertical orientation, demonstrating the similarity between the σ, π -donor frontier orbitals of the ligands NMe_2 and X_2CNMe_2 in 4 and 6 or 7 resp.
RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:503003 CAPLUS
DN 131:257662
TI Formation of Tantalum "Tuck-in" Complexes by Activation of Methyl C-H Bonds in Pentamethylcyclopentadiene Groups by Carbazole Ligation
AU Riley, Patrick N.; Parker, Jennifer R.; Fanwick, Phillip E.; Rothwell, Ian P.
CS Department of Chemistry, Purdue University, West Lafayette, IN, 47907-1393, USA
SO Organometallics (1999), 18(18), 3579-3583
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
OS CASREACT 131:257662
GI



AB The reaction of $[\text{Cp}^*\text{TaCl}_4]$ with the K salt of carbazole (cbK, >3 equiv) in hydrocarbon solvents leads to $[(\text{C}_5\text{Me}_4\text{CH}_2)\text{Ta}(\text{cb})_2\text{Cl}]$ (1; shown as I, R = cb), in which one of the ring Me C-H bonds of the Cp^* ligand was cleaved along with free cbH. Spectroscopic and structural studies of 1 show a lack of a plane of symmetry through the mol. with nonequivalent cb ligands. A minor component of the reaction mixture is believed to be the substitutional isomer in which both carbazole ligands are equivalent. Alkylation of 1 with $\text{LiCH}_2\text{SiMe}_3$ or PhCH_2MgCl generates the corresponding monoalkyl derivs. $[(\text{C}_5\text{Me}_4\text{CH}_2)\text{Ta}(\text{cb})_2(\text{R})]$ (7 or 8, resp.). Structural studies of 1, 7, and 8 support an $\eta^1:\eta^5\text{-CH}_2\text{C}_5\text{Me}_4$ ($\sigma:\eta^5\text{-CH}_2\text{C}_5\text{Me}_4$) description for the metalated ligands, with significant slippage toward an $\eta^1:\eta^3\text{-CH}_2\text{C}_5\text{Me}_4$ resonance form. To compare the extent of π -bonding between cb and dialkylamido ligands, $[(\text{cb})_2\text{Ta}(\text{NMe}_2)_3]$ (9) was synthesized and structurally characterized. The mol. structure of 9 consists of a tbp arrangement of N atoms with trans, axial cb ligands. The Ta-cb distances are 0.2 Å longer than the Ta-NMe₂ distances. An improved (safer) procedure for the synthesis of $[\text{Ta}(\text{NMe}_2)_5]$ is presented.

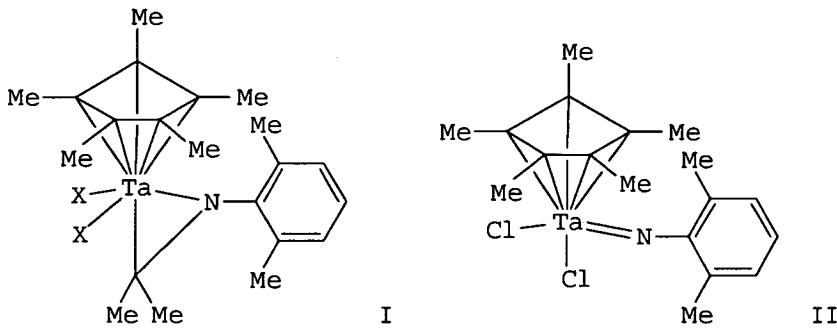
RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:577563 CAPLUS
DN 129:247356
TI Reduced Variational Space Analysis of Methane Adducts
AU Cundari, Thomas R.; Klinckman, Thomas R.
CS Department of Chemistry, The University of Memphis, Memphis, TN, 38152-6060, USA
SO Inorganic Chemistry (1998), 37(20), 5399-5401
CODEN: INOCAJ; ISSN: 0020-1669
PB American Chemical Society
DT Journal
LA English
AB An anal. of the binding of methane to transition metal complexes using the RVS-SCF (Reduced Variational Space-Self Consistent Field) technique was reported in order to optimize binding of methane to transition metal complexes for selective functionalization. Three energetic components dominate the binding of methane to the metal complex: Coulomb and exchange repulsion, polarization of methane, and charge transfer from methane to the metal complex. While the latter two are stabilizing interactions, energetic changes in the Coulomb and exchange repulsion are largely counterbalanced by changes in the methane polarization component. Trends as a function of metal, ligand, and charge on the methane binding energy are largely due to changes in the degree of charge transfer from methane to the metal complex.

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:409552 CAPLUS
DN 121:9552

TI Insertion of CNAr into Ta-Me bonds of TaCp*Cl_nMe_{4-n} (n = 0-3): intramolecular rearrangements, dynamic behavior, and x-ray crystal structure of TaCp*Cl₂(NAr) (Ar = 2,6-Me₂C₆H₃)
AU Galakhov, Mikhail V.; Gomez, Manuel; Jimenez, Gerardo; Pellinghelli, Maria Angela; Royo, Pascual; Tiripicchio, Antonio
CS Departamento de Quimica Inorganica, Universidad de Alcala, Alcala de Henares, E-28871, Spain
SO Organometallics (1994), 13(5), 1564-6
CODEN: ORGND7; ISSN: 0276-7333
DT Journal
LA English
OS CASREACT 121:9552
GI



AB The dimethyltantalum complex $TaCp^*Cl_2Me_2$ ($Cp^* = \eta^5-C_5Me_5$) reacts readily with isocyanide, $CNAr$ ($Ar = 2,6-Me_2C_6H_3$), to form the azatantalacyclopropane derivative $TaCp^*Cl_2(\eta^2-NArCMe_2)$ (1; shown as I, $X = Cl$), which can be alkylated with 2 equiv $LiMe$ to give the di-Me complex $TaCp^*Me_2(\eta^2-NArCMe_2)$ (2; shown as I, $X = Me$). Reaction of 1 and 2 with an addnl. 1 equiv of isocyanide leads to the imido complexes $TaCp^*Cl_2(NAr)$ (3; shown as II) and $TaCp^*Me(NArCMe:CMe_2)(NAr)$ (5), resp. Complex 5 is also obtained by reaction of $TaCp^*Me_4$ with 2 equiv of isocyanide, and the same reaction with $TaCp^*ClMe_3$ leads to $TaCp^*Cl(NArCMe:CMe_2)(NAr)$ (4). The complexes were characterized by NMR studies (1H, 13C, and 13C CP/MAS), and the crystal structure of complex 3 was determined by x-ray crystallog. The dynamic behavior of complexes 1, 2, 4, and 5 was studied in solution, and kinetic parameters were calculated from 1H DNMR data.

L1 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1993:51166 CAPLUS

DN 118:51166

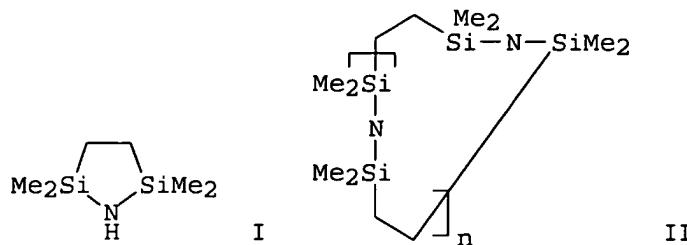
TI Multiple bonds between main group elements and transition metals. CXX.
. Niobium and **tantalum amide** complexes and new
cyclocarbodisilazanes

AU Herrmann, Wolfgang A.; Dvckhoff, Florian; Herdtweck, Eberhardt
CS Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, D-8046, Germany
SO Chemische Berichte (1992), 125(12), 2651-6
CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

GI



AB L3M:O (M = Nb, Ta; HL = I) are accessible by the reaction of MOC13 with LLi in 30 and 19% isolated yield, resp. The new silazanes II (n = 2, 3) are prepared from Me2ClSiCH2CH2SiClMe2 and NH3. The structures of II (n = 2, 3) were determined by single-crystal structure analyses.

L1 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:128189 CAPLUS

DN 114:128189

TI Tantalum amide preparation

AU Chestnut, Robert W.; Rothwell, Ian P.; Holl, Mark Banaszak; Wolczanski, Peter T.

CS Purdue Univ., IN, USA

SO Chemical & Engineering News (1990), 68(31), 2

CODEN: CENEAR; ISSN: 0009-2347

DT Journal

LA English

AB Explosions of LiNMe2-TaCl5 mixts. can be avoided in the preparation of pentakisdimethylamidotantalum by the TaCl5 addition to a slurry of LiNMe2 in pentane method by D. C. Bradley and M. Thomas, Can. J. Chemical, 40, 1355 (1962). LiNMe2 should be prepared in situ using excess HNMe2. The reaction will proceed smoothly using a pentane/diethyl ether solvent mixture (50/50).

L1 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1988:476196 CAPLUS

DN 109:76196

TI Transition metal carbides and process for making same

IN Laine, Richard M.

PA SRI International, USA

SO PCT Int. Appl., 18 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 4

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|--|------|----------|-----------------|----------|
| PI | WO 8801603 | A1 | 19880310 | WO 1987-US2057 | 19870820 |
| | W: JP | | | | |
| | RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE | | | | |
| | EP 278970 | A1 | 19880824 | EP 1987-905851 | 19870820 |
| | EP 278970 | B1 | 19930407 | | |
| | R: BE, DE, FR, GB, IT, NL | | | | |
| | JP 01502427 | T2 | 19890824 | JP 1987-505447 | 19870820 |
| | CA 1313938 | A1 | 19930302 | CA 1987-545246 | 19870825 |

PRAI US 1986-900592 A 19860826
WO 1987-US2057 W 19870820

OS MARPAT 109:76196

AB The title carbides are manufactured by a process comprising pyrolyzing a tractable transition metal amide of the formula $M_x(NR_1R_2)_y$ ($M = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Hf, Ta, W, Re, Os, Ir, Pt$, and all elements having atomic no ≥ 89 ; $x \geq 2$; $R_1, 2 = H$, lower alkyl, trimethylsilyl, C_2H_4 , but cannot both be H; $Y = \text{integer equal to valence of } M_x$), under nonoxidizing conditions at a temperature at which a C-containing group or amido group of the amide undergoes chemical reactions with a metal atom of the amide to form ≥ 1 covalent C-metal bonds. These carbides are used in making a variety of hard and/or high-temperature materials at low temps. Ni-coated stainless steel tubes were charged with 0.07 g

W2(NMe2)6 under Ar, N, or NH3, and pyrolyzed at 800° for 25 min.
The product had the crystal structure of hexagonal W2C3.

L1 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1979:65850 CAPLUS
DN 90:65850
TI Structure and reactivity in the group 5B tert-butylimido complexes
(Me2N)3M=NCMe3; x-ray crystal and molecular structure of
N-tert-butylimidotris(dimethylamido)tantalum
AU Nugent, William A.; Harlow, Richard L.
CS Cent. Res. Dev. Dep., E. I. du Pont de Nemours and Co., Wilmington, DE,
USA
SO Journal of the Chemical Society, Chemical Communications (1978), (14),
579-80
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
AB MCl5 (M = Nb, Ta) reacted with LiNMe2 and LiNHCMe3 to give (Me2N)3M:NCMe3
which were characterized by NMR spectra and extended Hueckel MO calcns.
Ta(NMe2)5 with Me3CNH2 also gave (Me2N)3Ta:NCMe3. The complexes underwent
typical reactions of the dialkylamide ligands with electrophiles, e.g.
Ph2CO. There is a linear M:N-C unit in each complex; the M:N bond of 1.77
Å is the longest known. The crystal and mol. structure of
(Me2N)3Ta:NCMe3 was determined from x-ray diffractometer data by the heavy atom
method and refined by least squares to R 0.076 for 1017 observed reflections.
The Me groups of the NCMe3 moiety are disordered about the 3-fold axis.

(FILE 'HOME' ENTERED AT 12:47:42 ON 01 MAR 2005)

FILE 'CAPLUS' ENTERED AT 12:47:55 ON 01 MAR 2005

L1 17 S TANTALUM AMIDE

=> S "bis-diethylamino-tris-dimethylaminotantalum"

450536 "BIS"

30073 "DIETHYLAMINO"

114799 "TRIS"

0 "DIMETHYLAMINOTANTALUM"

0 "BIS-DIETHYLAMINO-TRIS-DIMETHYLAMINOTANTALUM"

("BIS" (W) "DIETHYLAMINO" (W) "TRIS" (W) "DIMETHYLAMINOTANTALUM")

L2